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2 Linear Models

2.1 General Linear Models

Any linear model can be written as

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1k} \\ x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & \vdots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nk} \end{bmatrix} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_k \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

$$\uparrow \qquad \uparrow \qquad \uparrow$$

observed responses

the elements of X are known

(non-random) values

random errors are not observed response variable

.

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For the i-th case, the observed values are

$$(y_i \quad x_{i1} \quad x_{i2} \quad \cdots \quad x_{ik})$$

$$\uparrow \qquad \qquad \uparrow$$

explanatory variables that describe conditions under which the response was generated.

where ϵ specifying the distribution of the random error vector completes the specification of the distribution of \mathbf{y}

Note:

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$$\epsilon = \mathbf{y} - \mathbf{X}\boldsymbol{\beta} = \mathbf{y} - E(\mathbf{y})$$

Then,

$$E(\epsilon) = \mathbf{0}$$

$$V(\epsilon) = V(\mathbf{y}) = \mathbf{\Sigma}$$

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Example 1. Regression Analysis: Yield of a chemical process

Yield (%) Temperature (${}^{o}F$) Time (hr)

y	x_1	x_2
77	160	1
82	165	3
84	165	2
89	170	1
94	175	2

Simple linear regression model

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i$$
$$i = 1, 2, 3, 4, 5$$

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Example 2.

Blood coagulation times (in seconds) for blood samples from six different rats. Each rat was fed one of three diets.

A "means" model

$$y_{ij} = \mu_i + \epsilon_{ij}$$

$$\nearrow \quad \uparrow \qquad \nwarrow$$
observed time mean time random error for the *j*-th for rats with rat fed the given the $E(\epsilon_{ij}) = 0$
 i -th diet i -th diet

Matrix formulation:

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0

You can express this model as

An "effects" model

$$y_{ij} = \mu + \alpha_i + \epsilon_{ij}$$

This can be expressed as

This is a linear model with

$$E(\mathbf{y}) = \mathbf{X} \boldsymbol{\beta}$$
 and $V(\mathbf{y}) = \Sigma$

You could add the assumptions

- independent errors
- \bullet homogeneous variance, i.e. $V(\epsilon_{ij}) = \sigma^2$

to obtain a linear model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$ with

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$$
 and $V(\mathbf{y}) = \sigma^2 \mathbf{I}$

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error

Example 3. A 2×2 factorial experiment

- Experimental units: 8 plots with 5 trees per plot.
- Factor 1: Variety (A or B)
- Factor 2: Fungicide use (new or old)
- Response: Percentage of apples with spots

Percentage of		Fungicide
apples with spots	Variety	use
$y_{111} = 4.6$	А	new
$y_{112} = 7.4$	Α	new
$y_{121} = 18.3$	A	old
$y_{122} = 15.7$	A	old
$y_{211} = 9.8$	В	new
$y_{212} = 14.2$	В	new
$y_{211} = 21.1$	В	old
$y_{222} = 18.9$	В	old

 $y_{ijk} = \mu + V_i + F_j + V F_{ij} + \epsilon_{ijk}$ $\uparrow \qquad \uparrow \qquad \uparrow \qquad \uparrow$ percent variety fung. inter- random

with effects use action spots (i=1,2) (j=1,2) (k=1,2)

Here we are using 9 parameters

 $\boldsymbol{\beta}^T = (\mu \ V_1 \ V_2 \ F_1 \ F_2 \ V F_{11} \ V F_{12} \ V F_{21} \ V F_{22})$

to represent the 4 response means,

 $E(y_{ijk}) = \mu_{ij}, \quad i = 1, 2, \text{ and } j = 1, 2,$

corresponding to the 4 combinations of levels of the two factors.

Write this model in the form

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

A "means" model

$$y_{ijk} = \mu_{ij} + \epsilon_{ijk}$$

where

 $\mu_{ij} = E(y_{ijk})$ = mean percentage of apples with spots. This linear model can be written in the form $\mathbf{v} = \mathbf{X} \boldsymbol{\beta} + \boldsymbol{\epsilon}$, that is,

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Gauss-Markov Model

Definition 1.

2.2

The linear model

$$\mathbf{y} = \mathbf{X} \boldsymbol{\beta} + \boldsymbol{\epsilon}$$

is a Gauss-Markov model if

$$V(\mathbf{y}) = V(\boldsymbol{\epsilon}) = \sigma^2 I$$

for an unknown constant $\sigma^2 > 0$.

Notation:
$$\mathbf{y} \curvearrowright (\mathbf{X} \boldsymbol{\beta}_{\mathbf{x}}, \sigma^2 I)$$
distributed $E(\mathbf{y}) \quad V(\mathbf{y})$

The distribution of \mathbf{y} is not completely specified.

The "effects" linear model and the "means" linear model are equivalent in the sense that the space of possible mean vectors

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$$

is the same for the two models.

- the model matrices differ
- the parameter vectors differ
- the columns of the model matrices span the same vector space

$$\begin{split} E(\mathbf{y}) &= \mathbf{X}\boldsymbol{\beta} \\ &= \begin{bmatrix} \mathbf{x}_1 \middle| \mathbf{x}_2 \middle| \cdots \middle| \mathbf{x}_k \end{bmatrix} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_k \end{bmatrix} \\ &= \beta_1 \, \mathbf{x}_1 + \beta_2 \, \mathbf{x}_2 + \cdots + \beta_k \, \mathbf{x}_k \end{split}$$

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Normal Theory Gauss-Markov Model 2.3

Definition 2.

A normal-theory Gauss-Markov model is a Gauss-Markov model in which \mathbf{y} (or $\boldsymbol{\epsilon}$) has a multivariate normal distribution.

$$\mathbf{y} \sim N \quad (\mathbf{X} \boldsymbol{\beta} , \sigma^2 I)$$
 $\nearrow \quad \uparrow \quad \nwarrow \quad \nwarrow$
distr. multivar. $E(\mathbf{y}) \quad V(\mathbf{y})$
as normal
distr.

The additional assumption of a normal distribution is

- not needed for some estimation results
- useful in creating
 - confidence intervals
 - tests of hypotheses

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2.4 Ordinary Least Squares Estimation

For the linear model with

$$E(\mathbf{y}) = \mathbf{X} \boldsymbol{\beta}$$
 and $V(\mathbf{y}) = \boldsymbol{\Sigma}$

we have

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} X_{11} & X_{12} & \cdots & X_{1k} \\ X_{21} & X_{22} & \cdots & X_{2k} \\ \vdots & \vdots & & \vdots \\ X_{n1} & X_{n2} & \cdots & X_{nk} \end{bmatrix} \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_k \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

and

$$y_i = \beta_1 \mathbf{x}_{i1} + \beta_2 \mathbf{x}_{i2} + \dots + \beta_k \mathbf{x}_{ik} + \epsilon_i$$

= $\mathbf{X}_i^T \boldsymbol{\beta} + \epsilon_i$

where $\mathbf{X}_{i}^{T} = (\mathbf{x}_{i1}, \mathbf{x}_{i2}, \cdots, \mathbf{x}_{ik})$ is the *i*-th row of the model matrix \mathbf{X} .

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These are often called the "normal" equations.

If $\mathbf{X}_{n \times k}$ has full column rank, i.e., rank $(\mathbf{X}) = k$, then

- $\mathbf{X}^T\mathbf{X}$ is non-singular
- $(\mathbf{X}^T\mathbf{X})^{-1}$ exists and is unique

Consequently,

$$(\mathbf{X}^T\mathbf{X})^{-1}(\mathbf{X}^T\mathbf{X})\mathbf{b} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$$

and

$$\mathbf{b} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{v}$$

is the unique solution to the normal equations.

If $rank(\mathbf{X}) < k$, then

- there are infinitely many solutions to the normal equations
- if $(\mathbf{X}^T\mathbf{X})^-$ is a generalized inverse of $\mathbf{X}^T\mathbf{X}$, then

$$\mathbf{b} = (\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T \mathbf{y}$$

is a solution of the normal equations.

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Definition 3.

For a linear model with $E(\mathbf{y}) = X\boldsymbol{\beta}$, any vector **b** that minimizes the sum of squared residuals

$$Q(\mathbf{b}) = \sum_{i=1}^{n} (y_i - \mathbf{X}_i^T \mathbf{b})^2$$
$$= (\mathbf{y} - X\mathbf{b})^T (\mathbf{y} - X\mathbf{b})^2$$

is an ordinary least squares (OLS) estimator for $\boldsymbol{\beta}$.

For $j = 1, 2, \ldots, k$, solve

$$0 = \frac{\partial Q(\mathbf{b})}{\partial b_j} = 2\sum_{i=1}^n (y_i - \mathbf{X}_i^T \mathbf{b}) X_{ij}$$

Dividing by 2, we have

$$0 = \sum_{i=1}^{n} (y_i - \mathbf{X}_i^T \mathbf{b}) X_{ij} \quad j = 1, 2, \dots, k$$

These equations are expressed in matrix form as

$$0 = \mathbf{X}^T(\mathbf{y} - \mathbf{X}\mathbf{b})$$
$$= \mathbf{X}^T\mathbf{y} - \mathbf{X}^T\mathbf{X}\mathbf{b}$$

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$$\mathbf{X}^T \mathbf{X} \mathbf{b} = \mathbf{X}^T \mathbf{y}$$

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Suppose that we are interested in the coefficients $\boldsymbol{\beta}$ of a linear model $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$, where \mathbf{Y} is $n \times 1$, \mathbf{X} is $n \times p$ and $\boldsymbol{\epsilon} \sim N(\mathbf{0}, \sigma^2 \mathbf{I})$. Furthermore, suppose that it is of interest to partition that model in the form $\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{X}_2 & \mathbf{X}_3 \end{bmatrix}$, for $n \times p_i$ matrices $\mathbf{X}_i, i = 1, 2, 3$. Finally, suppose that an investigator creates a partially orthogonal design, in which $\mathbf{X} = \begin{bmatrix} \mathbf{X}_1 & \mathbf{X}_2 & \mathbf{X}_3 \end{bmatrix}$ has the property that $\mathbf{X}_i^T \mathbf{X}_j = 0$ for $i \neq j$. Show that the least squares estimate of $\boldsymbol{\beta}$ takes the form $\hat{\boldsymbol{\beta}}$

the least squares
$$= \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \hat{\beta}_3 \end{bmatrix}, \text{ where}$$

Example 4.

$$\bullet \; \boldsymbol{\hat{\beta}}_1 = (\mathbf{X}_1^T \mathbf{X}_1)^{-1} \mathbf{X}_1^T \mathbf{Y}$$

$$\bullet \ \hat{\boldsymbol{\beta}}_2 = (\mathbf{X}_2^T \mathbf{X}_2)^{-1} \mathbf{X}_2^T \mathbf{Y}$$

$$\bullet \; \boldsymbol{\hat{\beta}_3} = (\mathbf{X_3^TX_3})^{-1}\mathbf{X_3^TY}$$

Generalized Inverse 2.5

Definition 4.

For a given $m \times n$ matrix **A**, any $n \times m$ matrix G that satisfies

$$AGA = A$$

is a **generalized inverse** of **A**.

Comments:

- (i) We will often use **A**⁻ to denote a generalized inverse of \mathbf{A} .
- (ii) There may be infinitely many generalized in-
- (iii) If **A** is an $m \times m$ nonsingular matrix, then $\mathbf{G} = \mathbf{A}^{-1}$ is the unique generalized inverse for **A**

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Example 5. $\mathbf{A} = \begin{bmatrix} 16 & -6 & -10 \\ -6 & 21 & -15 \\ -10 & -15 & 25 \end{bmatrix} \text{ with } \operatorname{rank}(\mathbf{A}) = 2.$ Check that

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Check that
$$\mathbf{G}_1 = \begin{bmatrix} \frac{1}{20} & 0 & 0 \\ 0 & \frac{1}{30} & 0 \\ 0 & 0 & \frac{1}{50} \end{bmatrix} \text{ and } \mathbf{G}_2 = \begin{bmatrix} \frac{21}{300} & \frac{6}{300} & 0 \\ \frac{6}{300} & \frac{16}{300} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

are generalized inverse of A

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Example 6.

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A "means" model is as follow:

$$\begin{bmatrix} y_{11} \\ y_{12} \\ y_{21} \\ y_{31} \\ y_{32} \\ y_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \mu_1 \\ \mu_2 \\ \mu_3 \end{bmatrix} + \begin{bmatrix} \epsilon_{11} \\ \epsilon_{12} \\ \epsilon_{21} \\ \epsilon_{31} \\ \epsilon_{32} \\ \epsilon_{33} \end{bmatrix}$$

- (i) Compute $\mathbf{X}^T\mathbf{X}$ and $\mathbf{X}^T\mathbf{y}$.
- (ii) Obtain the OLS estimator.

Example 7.

"Effects" model

$$y_{ij} = \mu + \alpha_i + \epsilon_{ij}$$

 $i = 1, 2, 3; j = 1, 2, \dots, n_i$

(i) Write out the $\mathbf{X}^T\mathbf{X}$ matrix for this models.

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(iii) Another generalized inverse for $\mathbf{X}^T\mathbf{X}$ is

$$(\mathbf{X}^T \mathbf{X})^- = \begin{bmatrix} \begin{bmatrix} n_1 & n_1 & n_2 \\ n_1 & n_1 & 0 \\ n_2 & 0 & n_2 \end{bmatrix}^{-1} & 0 \\ n_2 & 0 & n_2 \end{bmatrix}^{-1} & 0$$

Compute the corresponding solution to the normal equations.

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(ii) Check that $(\mathbf{X}^T \mathbf{X})^- = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{n_1} & 0 & 0 \\ 0 & 0 & \frac{1}{n_2} & 0 \\ 0 & 0 & 0 & \frac{1}{n_3} \end{bmatrix}$ is

a generalized inversed of $\mathbf{X}^T \mathbf{X}$ and compute the corresponding solution to the normal equations.

2.5.1**Evaluating Generalized Inverses**

- Step(1) Find any $r \times r$ nonsingular submatrix of **A** where $r=\operatorname{rank}(\mathbf{A})$. Call this matrix \mathbf{W} .
- Step(2) Invert and transpose \mathbf{W} , ie., compute $(\mathbf{W}^{-1})^T$.
- Step(3) Replace each element of W in A with the corresponding element of $(\mathbf{W}^{-1})^T$
- Step(4) Replace all other elements in **A** with ze-
- Step(5) Transpose the resulting matrix to obtain \mathbf{G} , a generalized inverse for \mathbf{A} .

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Example 8.
$$\mathbf{A} = \begin{bmatrix} 4 & 1 & 2 & 0 \\ 1 & \textcircled{1} & \textcircled{5} & 15 \\ 3 & \textcircled{1} & \textcircled{3} & 5 \end{bmatrix}$$

$$\mathbf{W} = \begin{bmatrix} 1 & 5 \\ 1 & 3 \end{bmatrix}$$

You are given that $rank(\mathbf{A}) = 2$, find $\mathbf{G} = \mathbf{A}^-$.

Example 9.

ample 9.
$$\mathbf{A} = \begin{bmatrix} \textcircled{4} & 1 & 2 & \textcircled{0} \\ 1 & 1 & 5 & 15 \\ \textcircled{3} & 1 & 3 & \textcircled{5} \end{bmatrix}$$

$$\mathbf{W} = \begin{bmatrix} 4 & 0 \\ 3 & 5 \end{bmatrix}$$

You are given that $rank(\mathbf{A}) = 2$, find $\mathbf{G} = \mathbf{A}^-$.

2.5.2 Moore-Penrose Inverse

Definition 5. For any matrix A there is a **unique** matrix M, called the Moore-Penrose inverse, that satisfies

- (i) $\mathbf{A}M\mathbf{A} = \mathbf{A}$
- (ii) $M\mathbf{A}M = M$
- (iii) $\mathbf{A}M$ is symmetric
- (iv) $M\mathbf{A}$ is symmetric

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2.5.3 Properties of generalized inverses of $\mathbf{X}^T\mathbf{X}$

Result 1. If **G** is a generalized inverse of $\mathbf{X}^T \mathbf{X}$, then

- (i) \mathbf{G}^T is a generalized inverse of $\mathbf{X}^T \mathbf{X}$.
- (ii) $\mathbf{X}\mathbf{G}\mathbf{X}^T\mathbf{X} = \mathbf{X}$, i.e., $\mathbf{G}\mathbf{X}^T$ is a generalized inverse of \mathbf{X} .
- (iii) \mathbf{XGX}^T is invariant with respect to the choice of \mathbf{G} .
- (iv) $\mathbf{X}\mathbf{G}\mathbf{X}^T$ is symmetric.

trix

Result 2. Properties of a projection ma-

 $P_{\mathbf{X}} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T$

(i) $P_{\mathbf{X}}$ is invariant to the choice of $(\mathbf{X}^T\mathbf{X})^-$

normal equations

 $P_{\mathbf{X}}\mathbf{X}_{i} = \mathbf{X}_{i}$

For any solution $\mathbf{b} = (\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T \mathbf{y}$ to the

 $\hat{\mathbf{y}} = \mathbf{X}\mathbf{b} = P_{\mathbf{X}}\mathbf{y}$

is the same. (From Result 1(iii))

(iii) $P_{\mathbf{X}}$ is idempotent $(P_X P_X = P_X)$

(iv) $P_X \mathbf{X} = \mathbf{X}$ (From Result 1 (ii))

(ii) $P_{\mathbf{X}}$ is symmetric (From Result 1 (iv))

(v) Partition **X** as $\mathbf{X} = [\mathbf{X}_1 | \mathbf{X}_2 | \cdots | \mathbf{X}_k]$, then

2.6 Estimation of the Mean Vector

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$$

For any solution to the normal equations, say

$$\mathbf{b} = (\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T \mathbf{y} ,$$

2.6.1 OLS Estimator E(y)

The OLS estimator for $E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$ is

$$\begin{split} \hat{\mathbf{y}} &= \mathbf{X}\mathbf{b} \\ &= \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-}\mathbf{X}^T\mathbf{y} \\ &= P_{\mathbf{X}}\mathbf{y} \end{split}$$

- The matrix $P_{\mathbf{X}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-}\mathbf{X}^T$ is called an "orthogonal projection matrix".
- $\hat{\mathbf{y}} = P_{\mathbf{X}}\mathbf{y}$ is the projection of \mathbf{y} onto the space spanned by the columns of \mathbf{X} .

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2.6.2 Residuals

$$\mathbf{e}_i = \mathbf{y}_i - \hat{\mathbf{y}}_i \quad i = 1, \dots, n$$

$$\begin{aligned} \mathbf{e} &= \mathbf{y} - \hat{\mathbf{y}} \\ &= \mathbf{y} - \mathbf{X}\mathbf{b} \\ &= \mathbf{y} - \mathbf{P}_{\mathbf{X}}\mathbf{y} \\ &= (\mathbf{I} - \mathbf{P}_{\mathbf{X}})\mathbf{y} \end{aligned}$$

Comment: $I - P_X$ is a projection matrix that projects y onto the space orthogonal to the space spanned by the columns of X.

Result 3.

- (i) $\mathbf{I} \mathbf{P}_{\mathbf{X}}$ is symmetric
- (ii) $\mathbf{I} \mathbf{P}_{\mathbf{X}}$ is idempotent

$$(I - P_X)(I - P_X) = I - P_X$$

(iii)
$$(\mathbf{I} - \mathbf{P}_{\mathbf{X}})\mathbf{P}_{\mathbf{X}} = 0$$

(iv)
$$(\mathbf{I} - \mathbf{P}_{\mathbf{X}})\mathbf{X} = \mathbf{0}$$

(v) Partition **X** as $[\mathbf{x}_1|\mathbf{x}_2|\cdots|\mathbf{x}_k]$ then

$$(\mathbf{I} - \mathbf{P}_{\mathbf{X}})\mathbf{X}_j = \mathbf{0}$$

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(vi) Residuals are invariant with respect to the choice of $(\mathbf{X}^T\mathbf{X})^-$, so

$$e - v - Xb = (I - P_X)v$$

is the same for any solution

$$\mathbf{b} = (\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T \mathbf{y}$$

to the normal equations

The residual vector

$$e = y - \tilde{y} = (I - P_X)y$$

is in the space orthogonal to the space spanned by the columns of X. It has dimension

$$n-rank(\mathbf{X}).$$

2.6.3 Partition of a total sum of squares

Squared length of \mathbf{y} is

$$\sum_{i=1}^{n} y_i^2 = \mathbf{y}^T \mathbf{y}$$

Squared length of the residual vector is

$$\begin{split} \sum_{i=1}^n e_i^2 &= \mathbf{e}^T \mathbf{e} \\ &= [(I - P_X)\mathbf{y}]^T (I - P_X)\mathbf{y} \\ &= \mathbf{y}^T (I - P_X)\mathbf{y} \end{split}$$

Squared length of $\hat{\mathbf{y}} = P_X \mathbf{y}$ is

$$\begin{split} \sum_{i=1}^n \hat{y}_i^2 &= \hat{\mathbf{y}}^T \hat{\mathbf{y}} \\ &= (P_X \mathbf{y})^T (P_X \mathbf{y}) \\ &= \mathbf{y}^T (P_X)^T P_X \mathbf{y} \quad \text{since } P_X \text{ is symmetric} \\ &= \mathbf{y}^T P_X P_X \mathbf{y} \quad \text{since } P_X \text{ is idempotent} \\ &= \mathbf{y}^T P_X \mathbf{y} \end{split}$$

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We have

$$\mathbf{y}^T \mathbf{y} = \mathbf{y}^T (P_X + I - P_X) \mathbf{y}$$
$$= \mathbf{y}^T P_X \mathbf{y} + \mathbf{y}^T (I - P_X) \mathbf{y}.$$

Analysis of Variance Table

Analysis of variance Table			
Source of	Degrees of	Sums of Squares	
Variation	Freedom		
model (un-	$rank(\mathbf{X})$	$ \hat{\mathbf{y}}^T \hat{\mathbf{y}} = \mathbf{y}^T P_X \mathbf{y}$	
corrected)			
residuals	$\operatorname{n-rank}(\mathbf{X})$	$\mathbf{e}^T \mathbf{e} = \mathbf{y}^T (I - P_X) \mathbf{y}$	
total (un- corrected)	n	$\mathbf{y}^T \mathbf{y} = \sum_{i=1}^n y_i^2$	

Result 4.

For the linear model with

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$$
 and $V(y) = \boldsymbol{\Sigma}$,

the OLS estimator

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{b} = P_X\mathbf{y}$$

for

 $X\beta$

is

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- (i) unbiased, i.e., $E(\hat{\mathbf{y}}) = \mathbf{X}\boldsymbol{\beta}$
- (ii) a linear function of **y**
- (iii) has variance-covariance matrix

$$V(\hat{\mathbf{y}}) = P_X \Sigma P_X$$

This is true for any solution

$$b = (\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T \mathbf{y}$$

to the normal equations.

-

Comments:

(i) $\hat{\mathbf{y}} = \mathbf{X}\mathbf{b} = P_X\mathbf{y}$ is said to be a **linear unbiased** estimator for $E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$

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(ii) For the Gauss-Markov model, $V(\mathbf{y}) = \sigma^2 I$ and

$$\begin{split} V(\hat{\mathbf{y}}) &= P_X(\sigma^2 I) P_X \\ &= \sigma^2 P_X P_X \\ &= \sigma^2 P_X \\ &= \sigma^2 \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T \end{split}$$

this is sometimes called the "hat" matrix.

2.7 Estimable Functions

Some estimates of linear functions of the parameters have the same value, regardless of which solution to the normal equations is used. These are called estimable functions.

Definition 6.

For a linear model with

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$$
 and $V(\mathbf{y}) = \boldsymbol{\Sigma}$

we will say that

$$\mathbf{c}^T \boldsymbol{\beta} = c_1 \beta_1 + c_2 \beta_2 + \dots + c_k \beta_k$$

is **estimable** if there exists a linear unbiased estimator $\mathbf{a}^T \mathbf{y}$ for $\mathbf{c}^T \boldsymbol{\beta}$, i.e., for some vector of constants \mathbf{a} , we have $E(\mathbf{a}^T \mathbf{y}) = \mathbf{c}^T \boldsymbol{\beta}$.

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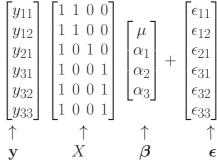
We will use **Blood coagulation times** example to illustrate estimable and non-estimable functions.

Diet 1	Diet 2	Diet 3
$y_{11} = 62$	$y_{21} = 71$	$y_{31} = 72$
$y_{12} = 60$		$y_{32} = 68$
		$y_{33} = 67$

The "Effects" model

$$y_{ij} = \mu + \alpha_i + \epsilon_{ij}$$

can be written as



Note that

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$$
 or $E(\boldsymbol{\epsilon}) = 0$

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2.7.1 Example of Estimable Functions

Example 10.

Show that $\mu + \alpha_1$ is estimable.

Example 11.

Show that $\mu + \alpha_2$ is estimable.

Example 12.

Show that $\mu + \alpha_3$ is estimable.

Show that $\alpha_1 - \alpha_2$ is estimable.

Example 13.

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Example 14.

Show that $2\mu + 3\alpha_1 - \alpha_2$ is estimable.

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2.7.2Quantities that are not estimable

Quantities that are **not** estimable include

$$\mu, \alpha_1, \alpha_2, \alpha_3, 3\alpha_1, 2\alpha_2$$

To show that a linear function of parameters

$$c_0\mu + c_1\alpha_1 + c_2\alpha_+c_3\alpha_3$$

is not estimable, one must show that there is no non-random vector

$$\mathbf{a^T} = (a_0, a_1, a_2, a_3)$$

For which

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$$E(\mathbf{a}^{\mathbf{T}}\mathbf{y}) = c_0\mu + c_1\alpha_1 + c_2\alpha_2 + c_3\alpha_3$$

Example 15.

Show that α_1 is not estimable.

Result 5.

For a model with $E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$ and $V(y) = \boldsymbol{\Sigma}$:

- (i) The expectation of any observation is estimable.
- (ii) A linear combination of estimable functions is estimable.
- (iii) Each element of β is estimable if and only if $\operatorname{rank}(\mathbf{X}) = k = \text{number of columns}$.
- (iv) Every $\mathbf{c}^T \boldsymbol{\beta}$ is estimable if and only if rank(\mathbf{X}) = $k = \text{number of columns in } \mathbf{X}$.

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Result 6. For a linear model with $E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$ and $V(\mathbf{y}) = \Sigma$, each of the following is true if and only if $\mathbf{c}^T \boldsymbol{\beta}$ is **estimable**.

- (i) $\mathbf{c}^T = \mathbf{a}^T \mathbf{X}$ for some \mathbf{a} i.e., \mathbf{c} is in the space spanned by the rows of \mathbf{X} .
- (ii) $\mathbf{c}^T \mathbf{a} = 0$ for every \mathbf{a} for which $\mathbf{X} \mathbf{a} = \mathbf{0}$.
- (iii) $\mathbf{c}^T \mathbf{b}$ is the same for any solution to the normal equations $(\mathbf{X}^T \mathbf{X}) \mathbf{b} = \mathbf{X}^T \mathbf{y}$, i.e., there is a **unique** least squares estimator for $\mathbf{c}^T \boldsymbol{\beta}$.

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Example 16.

Use Result 6 (ii) to show that μ is not estimable.

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Part (ii) of Result 6 sometimes provides a convenient way to identify all possible estimable functions of β .

In Blood Coagulation Times example,

$$Xd = 0$$

if and only if

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$$\mathbf{d} = w \begin{bmatrix} 1 \\ -1 \\ -1 \\ -1 \end{bmatrix}$$

for some scalar w.

Then,

$$\mathbf{c}^T \boldsymbol{\beta}$$

is estimable if and only if

$$0 = \mathbf{c}^T \mathbf{d} = w(c_1 - c_2 - c_3 - c_4) = 0$$

$$\iff c_1 = c_2 + c_3 + c_4.$$

Then.

 $(c_2+c_3+c_4)\mu+c_2\alpha_1+c_3\alpha_2+c_4\alpha_3$

is estimable for any $(c_2 \ c_3 \ c_4)$ and these are the only estimable functions of $\mu, \alpha_1, \alpha_2, \alpha_3$.

For example, some estimable functions are

$$\mu + \frac{1}{3}(\alpha_1 + \alpha_2 + \alpha_3) \quad (c_2 = c_3 = c_4 = \frac{1}{3})$$

and

$$\mu + \alpha_2$$
 $(c_2 = 1 \ c_3 = c_4 = 0)$

but

$$\mu + 2\alpha_2$$

is not estimable

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Example 18. Consider the model

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 $y_{ijk} = \mu + \alpha_i + \beta_j + \epsilon_{ijk}, i = 1, 2; j = 1, 2; k = 1.$

Describe the set of estimable functions of μ , α 's and β 's.

Example 17.

Let

$$\mathbf{y} = \begin{bmatrix} 1 & 0 \\ 1 & 0 \\ 0 & 1 \\ 1 & 1 \\ 1 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \\ \epsilon_6 \end{bmatrix}$$

Show that every linear parametric function $c_1\beta_1 + c_2\beta_2$ is estimable.

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Definition 7.

For a linear model with $E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$ and $V(\mathbf{y}) = \Sigma$, where **X** is an $n \times k$ matrix, $C_{r \times k}\boldsymbol{\beta}_{k \times 1}$ is said to be **estimable** if all of its elements

$$C\boldsymbol{\beta} = \begin{bmatrix} \mathbf{c}_1^T \\ \mathbf{c}_2^T \\ \vdots \\ \mathbf{c}_r^T \end{bmatrix} \boldsymbol{\beta} = \begin{bmatrix} \mathbf{c}_1^T \boldsymbol{\beta} \\ \mathbf{c}_2^T \boldsymbol{\beta} \\ \vdots \\ \mathbf{c}_r^T \boldsymbol{\beta} \end{bmatrix}$$

are estimable.

Result 7.

For the linear model with $E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$ and $V(\mathbf{y}) = \Sigma$, where **X** is an $n \times k$ matrix. Each of the following conditions hold if and only if $C\boldsymbol{\beta}$ is estimable.

- (i) $\mathbf{A}^T \mathbf{X} = C$ for some matrix \mathbf{A} , i.e., each row of C is in the space spanned by the rows of \mathbf{X} .
- (ii) $C\mathbf{d} = \mathbf{0}$ for any \mathbf{d} for which $\mathbf{X}\mathbf{d} = \mathbf{0}$.
- (iii) $C\mathbf{b}$ is the same for any solution to the normal equations $(\mathbf{X}^T\mathbf{X})\mathbf{b} = \mathbf{X}^T\mathbf{v}$.

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Here "best" means smallest expected squared error. Let $t(\mathbf{y})$ denote a linear unbiased estimator for $\mathbf{c}^T \boldsymbol{\beta}$. Then, the expected squared error is

$$\begin{aligned} \text{MSE} &= E[t(\mathbf{y}) - \mathbf{c}^T \boldsymbol{\beta}]^2 \\ &= E[t(\mathbf{y}) - E(t(\mathbf{y})) + E(t(\mathbf{y})) - \mathbf{c}^T \boldsymbol{\beta}]^2 \\ &= E[t(\mathbf{y}) - E(t(\mathbf{y}))]^2 \\ &+ [E(t(\mathbf{y})) - \mathbf{c}^T \boldsymbol{\beta}]^2 \\ &+ 2[E(t(\mathbf{y})) - \mathbf{c}^T \boldsymbol{\beta}] E[t(\mathbf{y}) - E(t(\mathbf{y}))] \\ &= E[t(\mathbf{y}) - E(t(\mathbf{y}))]^2 + [E(t(\mathbf{y})) - \mathbf{c}^T \boldsymbol{\beta}]^2 \\ &= V(t(\mathbf{y})) + [\text{bias}]^2 \end{aligned}$$

2.8 Best Linear Unbiased Estimator

For a linear model

$$y = X\beta + \epsilon$$

with

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$$
 and $V(\mathbf{y}) = \boldsymbol{\Sigma}$,

we have

- Any estimable function has a specific interpretation
- The OLS estimator for an estimable function $C\beta$ is unique

$$C\mathbf{b} = C(\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T \mathbf{y}$$

- ullet The OLS estimator for an estimable function $Coldsymbol{eta}$ is
 - a linear estimator
 - an unbiased estimator

In the class of linear unbiased estimators for $\mathbf{c}^T \boldsymbol{\beta}$, is the OLS estimator the "best?"

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We are restricting our attention to linear unbiased estimators for $\mathbf{c}^T \boldsymbol{\beta}$:

 $\bullet \ E(t(\mathbf{y})) = \mathbf{c}^T \boldsymbol{\beta}$

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• $t(\mathbf{y}) = \mathbf{a}^T \mathbf{y}$ for some \mathbf{a}

Then, $t(\mathbf{y}) = \mathbf{a}^T \mathbf{y}$ is the **Best Linear Unbiased Estimator (BLUE)** for $\mathbf{c}^T \boldsymbol{\beta}$ if

$$V(\mathbf{a}^T\mathbf{y}) \le V(\mathbf{d}^T\mathbf{y})$$

for any \mathbf{d} and any value of $\boldsymbol{\beta}$.

Result 8. Gauss-Markov Theorem

For the Gauss-Markov model with

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$$
 and $V(\mathbf{y}) = \sigma^2 I$

the OLS estimator of an estimable function $\mathbf{c}^T \boldsymbol{\beta}$ is the **unique** best linear unbiased estimator (blue) of $\mathbf{c}^T \boldsymbol{\beta}$.

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Example 19.

The response time in milliseconds was determined for three different types of circuits that could be used in an automatic valve shutoff mechanism. The results are shown in the following table.

Circuit Type	Re	espo	nse	Tir	ne
1	9	12	10	8	15
2	20	21	23	17	30
3	6	5	8	16	7

Consider the model

$$y_{ij} = \mu + \tau_i + \epsilon_{ij}$$
; $i = 1, 2, 3$; $j = 1, 2, 3, 4, 5$

where μ is the overall mean, τ_i is the circuit type content effects and $\epsilon_{ij} \sim N(0, \sigma^2)$ is the random error. Compute the BLUE of of $\tau_1 - 2\tau_2 + \tau_3$

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2.9 Generalized Least Squares (GLS) Estimation

What if you have a linear model that is **not** a Gauss-Markov model?

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$$
$$V(\mathbf{y}) = \Sigma \neq \sigma^2 I$$

• Parts (i) and (ii) of the proof of result 8 do not require

 $V(\mathbf{v}) = \sigma^2 I$.

Consequently, the OLS estimator for $\mathbf{c}^T \boldsymbol{\beta}$,

$$\mathbf{c}^T \mathbf{b} = \mathbf{c}^T (\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T \mathbf{v}$$

is a linear unbiased estimator.

• Result 6 does not require

$$V(\mathbf{y}) = \sigma^2 I$$

and the OLS estimator for any estimable quantity,

$$\mathbf{c}^T \mathbf{b} = \mathbf{c}^T (\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T \mathbf{y} ,$$

is invariant to the choice of $(\mathbf{X}^T\mathbf{X})^-$.

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Chapter 2 Linear Models 75 • The OLS estimator $\mathbf{c}^T \mathbf{b}$ may not be blue. There may be other linear unbiased estimators with smaller variance.

Note

$$V(\mathbf{c}^T \mathbf{b}) = V(\mathbf{c}^T (\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T \mathbf{y})$$
$$= \mathbf{c}^T (\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T \Sigma \mathbf{X} [(\mathbf{X}^T \mathbf{X})^{-}]^T \mathbf{c}$$

For the Gauss-Markov model

$$V(\mathbf{y}) = \Sigma = \sigma^2 I$$

and

$$V(\mathbf{c}^T \mathbf{b}) = \sigma^2 \mathbf{c}^T (\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T \mathbf{X} [(\mathbf{X}^T \mathbf{X})^{-}]^T \mathbf{c}$$
$$= \sigma^2 \mathbf{c}^T (\mathbf{X}^T \mathbf{X})^{-} \mathbf{c}$$

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$$
$$V(\mathbf{y}) = \Sigma \neq \sigma^2 I$$

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Then

$$V(\mathbf{Z}) = V(\Sigma^{-1/2}\mathbf{y})$$

$$= \Sigma^{-1/2}\Sigma \Sigma^{-1/2}$$

$$= I$$

and

$$E(\mathbf{Z}) = E(\Sigma^{-1/2}\mathbf{y})$$

$$= \Sigma^{-1/2}E(\mathbf{y})$$

$$= \Sigma^{-1/2}\mathbf{X}\boldsymbol{\beta}$$

$$= \mathbf{W}\boldsymbol{\beta}$$

and we have a Gauss-Markov model for \mathbf{Z} , where $\mathbf{W} = \Sigma^{-1/2}\mathbf{X}$ is the model matrix.

Note that

$$(\mathbf{Z} - \mathbf{W}\mathbf{b})^{T}(\mathbf{Z} - \mathbf{W}\mathbf{b})$$

$$= (\Sigma^{-1/2}\mathbf{y} - \Sigma^{1/2}\mathbf{X}\mathbf{b})^{T}(\Sigma^{-1/2}\mathbf{y}\Sigma^{-1/2}\mathbf{X}\mathbf{b})$$

$$= (y - \mathbf{X}\mathbf{b})^{T}\Sigma^{-1/2}\Sigma^{-1/2}(y - \mathbf{X}\mathbf{b})$$

$$= (y - \mathbf{X}\mathbf{b})^{T}\Sigma^{-1}(y - \mathbf{X}\mathbf{b})$$

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Definition 8.

For a linear model with

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$$
 and $V(\mathbf{y}) = \Sigma$,

where Σ is positive definite, a generalized least squares estimator for $\boldsymbol{\beta}$ minimizes

$$(\mathbf{y} - \mathbf{X}\mathbf{b}_{\text{gls}})^T \Sigma^{-1} (\mathbf{y} - \mathbf{X}\mathbf{b}_{\text{gls}})$$

Strategy: Transform \mathbf{y} to a random vector \mathbf{Z} for which the Gauss-Markov model applies. The spectral decomposition of Σ yields

$$\Sigma = \sum_{j=1}^{n} \lambda_j \mathbf{u}_j \mathbf{u}_j^T.$$

Define

$$\Sigma^{-1/2} = \sum_{j=1}^{n} \frac{1}{\sqrt{\lambda_j}} \mathbf{u}_j \mathbf{u}_j^T$$

and create the random vector $\mathbf{Z} = \Sigma^{-1/2}\mathbf{y}$.

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Hence, any GLS estimator for the \mathbf{y} model is an OLS estimator for the \mathbf{Z} model.

It must be a solution to the normal equations for the ${\bf Z}$ model

$$\mathbf{W}^T \mathbf{W} \mathbf{b} = \mathbf{W}^T \mathbf{Z}$$

$$\Leftrightarrow (\mathbf{X}^T \Sigma^{-1/2} \Sigma^{-1/2} \mathbf{X}) \mathbf{b}$$
$$= \mathbf{X}^T \Sigma^{-1/2} \Sigma^{-1/2} \mathbf{y}$$

$$\Leftrightarrow (\mathbf{X}^T \Sigma^{-1} \mathbf{X}) \mathbf{b} = \mathbf{X}^T \Sigma^{-1} \mathbf{y}$$

These are the generalized least squares estimating equations.

Any solution

$$\mathbf{b}_{\text{GLS}} = (\mathbf{W}^T \mathbf{W})^{-} \mathbf{W}^T \mathbf{Z}$$
$$= (\mathbf{X}^T \Sigma^{-1} \mathbf{X})^{-} \mathbf{X}^T \Sigma^{-1} \mathbf{y}$$

is called a generalized least squares (GLS) estimator for $\boldsymbol{\beta}$.

Result 9.

For the linear model with $E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$ and $V(\mathbf{y}) = \Sigma$ the GLS estimator of an estimable function $\mathbf{c}^T\boldsymbol{\beta}$,

$$\mathbf{c}^T\mathbf{b}_{\mathrm{GLS}} = \mathbf{c}^T(\mathbf{X}^T\Sigma^{-1}\mathbf{X})^{-}\mathbf{X}^T\Sigma^{-1}\mathbf{y} \ ,$$

is the unique blue of $\mathbf{c}^T \beta$.

Comments:

• For the linear model with

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$$
 and $V(\mathbf{y}) = \Sigma$

both the OLS and GLS estimators for an estimable function $\mathbf{c}^T \boldsymbol{\beta}$ are linear unbiased estimators.

$$V(\mathbf{c}^T \mathbf{b}_{\text{OLS}}) = \mathbf{c}^T (\mathbf{X}^T \mathbf{X})^{-} \mathbf{X}^T \Sigma \mathbf{X} [(\mathbf{X}^T \mathbf{X})^{-}]^T \mathbf{c}$$

$$V(\mathbf{c}^T \mathbf{b}_{\text{GLS}}) = \mathbf{c}^T (\mathbf{X}^T \Sigma^{-1} \mathbf{X})^{-1} \mathbf{X}^T \Sigma^{-1} \mathbf{X} (\mathbf{X}^T \Sigma^{-1} \mathbf{X})^{-1} \mathbf{c}$$

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 $\mathbf{c}^T \mathbf{b}_{\text{OLS}}$ is not a "bad" estimator, but $V(\mathbf{c}^T \mathbf{b}_{\text{OLS}}) \geq V(\mathbf{c}^T \mathbf{b}_{\text{GLS}})$

because $\mathbf{c}^T \mathbf{b}_{\text{GLS}}$ is the unique blue for $\mathbf{c}^T \boldsymbol{\beta}$.

• For the Gauss-Markov model,

$$\mathbf{c}^T b_{\text{GLS}} = \mathbf{c}^T b_{\text{OLS}} .$$

- The results for \mathbf{b}_{GLS} and $\mathbf{c}^T \mathbf{b}_{\text{GLS}}$ assume that $V(\mathbf{y}) = \mathbf{\Sigma}$ is known.
- The same results, hold for the model where $E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$ and $V(\mathbf{y}) = \sigma^2 V$ for some known matrix V.
- In practice $V(\mathbf{y}) = \Sigma$ is usually unknown. Then an approximation to

$$\mathbf{b}_{\mathrm{GLS}} = (\mathbf{X}^T \mathbf{\Sigma}^{-1} \mathbf{X})^{-} \mathbf{X}^T \mathbf{\Sigma}^{-1} \mathbf{y}$$

is obtained by substituting a consistent MEME16203 LINEAR MODELS

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estimator $\hat{\Sigma}$ for Σ .

— use method of moments or maximum likelihood estimation to obtain $\hat{\Sigma}$

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- the resulting estimator
 - * is not a linear estimator
 - * is consistent but not necessarily unbiased
 - * does not provide a blue for estimable functions
 - * may have larger mean squared error than the OLS estimator

To create confidence intervals or test hypotheses about estimable functions for a linear model with

$$E(\mathbf{y}) = \mathbf{X}\boldsymbol{\beta}$$
 and $V(\mathbf{y}) = \boldsymbol{\Sigma}$

we must

(i) specify a probability distribution for \mathbf{y} so we can derive a distribution for

$$\mathbf{c}^T \mathbf{b} = \mathbf{c}^T (\mathbf{X}^T \mathbf{\Sigma}^{-1} \mathbf{X})^{-1} \mathbf{X}^T \mathbf{\Sigma}^{-1} \mathbf{y}$$

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(ii) estimate σ^2 when

$$V(\mathbf{y}) = \sigma^2 I \text{ or } V(\mathbf{y}) = \sigma^2 V$$

for some known V.

(iii) Estimate Σ when

$$V(\mathbf{y}) = \mathbf{\Sigma}$$

Example 20.

Suppose that y_{11} and y_{12} are independent $N(\mu_1, \eta)$ variables independent of y_{21} and y_{21} that are independent $N(\mu_2, 4\eta)$ variables. (The η and 4η are variances.) What is the BLUE of $\mu_1 - \mu_2$? Explain carefully.

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Example 21.

Suppose $y_i = \beta_0 + \beta_1 x_i + \epsilon_i$, where for $\epsilon = (\epsilon_1, \epsilon_2, \dots, \epsilon_n)'$, $E(\epsilon) = \mathbf{0}$. A particular experiment produces n = 5 data points as per table below:

Suppose that $V(\epsilon) = \sigma^2 diag(1, 4, 9, 25)$.

(i) Give a matrix **T** such that **Ty** follows a Gauss- Markov model.

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(ii) What is the model matrix for $\mathbf{T}\mathbf{y}$?

(iii) Evaluate an appropriate point estimate of β under these model assumptions.

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2.10 Reparameterization, Restrictions, and Avoiding Generalized Inverses

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Models that may appear to be different at first sight, may be equivalent in many ways.

Example 22. Two-way classification Consider the "cell mean" model.

$$y_{ijk} = \mu_{ij} + \epsilon_{ijk} \ i = 1, 2; j = 1, 2; k = 1, 2$$

where $\epsilon_{ijk} \sim NID(0, \sigma^2)$

$$\begin{bmatrix} y_{111} \\ y_{112} \\ y_{121} \\ y_{122} \\ y_{211} \\ y_{212} \\ y_{221} \\ y_{222} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ y_{222} \end{bmatrix} + \begin{bmatrix} \epsilon_{111} \\ \epsilon_{112} \\ \epsilon_{121} \\ \mu_{11} \\ \mu_{12} \\ \mu_{21} \\ \mu_{21} \\ \mu_{22} \end{bmatrix} + \begin{bmatrix} \epsilon_{111} \\ \epsilon_{122} \\ \epsilon_{211} \\ \epsilon_{212} \\ \epsilon_{221} \\ \epsilon_{222} \end{bmatrix}$$

or

 $y = W\gamma + \epsilon$

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The "effects" model:

$$y_{ijk} = \mu + \alpha_i + \beta_j + \gamma_{ij} + \epsilon_{ijk}$$

where

$$\epsilon_{ijk} \sim NID(0, \sigma^2)$$
 1 = 1, 2; j = 1, 2; k = 1, 2

or

$$\mathbf{v} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

The models are "equivalent": the space spanned by the columns of \mathbf{W} is the same as the space spanned by columns of X.

You can find matrices F and G such that

and

$$X = \mathbf{W} \begin{bmatrix} 1 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 \end{bmatrix} = \mathbf{WG}$$

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Example 23. Regression model for the yield of a chemical process

$$y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \epsilon_i$$

$$\uparrow \qquad \uparrow \qquad \uparrow$$
yield temperature time

An "equivalent" model is

$$y_i = \alpha_0 + \beta_1 (X_{1i} - \bar{X}_{1.}) + \beta_2 (X_{2i} - \bar{X}_{2.}) + \epsilon_i$$

For the first model:

$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix} = \begin{bmatrix} 1 & X_{11} & X_{21} \\ 1 & X_{12} & X_{22} \\ 1 & X_{13} & X_{23} \\ 1 & X_{14} & X_{24} \\ 1 & X_{15} & X_{25} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \end{bmatrix} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

Then,

(i)
$$\operatorname{rank}(X) = \operatorname{rank}(\mathbf{W})$$

(ii) Estimated mean responses are the same:

$$\begin{aligned} \hat{\mathbf{y}} &= X(X^TX)^-X^T\mathbf{y} \\ &= \mathbf{W}(\mathbf{W}^T\mathbf{W})^{-1}\mathbf{W}^T\mathbf{y} \end{aligned}$$

or

$$\hat{\mathbf{y}} = P_X \mathbf{y} = P_{\mathbf{W}} \mathbf{y}$$

(iii) Residual vectors are the same

$$\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}} = (I - P_X)\mathbf{y}$$
$$= (I - P_\mathbf{W})\mathbf{y}$$

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For the second model:

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$$\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix} \begin{bmatrix} 1 & X_{11} - \bar{X}_1 & X_{21} - \bar{X}_2 \\ 1 & X_{12} - \bar{X}_1 & X_{22} - \bar{X}_2 \\ 1 & X_{13} - \bar{X}_1 & X_{23} - \bar{X}_2 \\ 1 & X_{14} - \bar{X}_1 & X_{24} - \bar{X}_2 \\ 1 & X_{15} - \bar{X}_1 & X_{25} - \bar{X}_2 \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \beta_1 \\ \beta_2 \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \end{bmatrix} = \mathbf{W} \boldsymbol{\gamma} + \boldsymbol{\epsilon}$$

The space spanned by the columns of X is the same as the space spanned by the columns of \mathbf{W} . Find matrices \mathbf{G} and F such that $X = \mathbf{W}\mathbf{G}$ and $\mathbf{W} = XF$.

Definition 9.

Consider two linear models:

1.
$$E(\mathbf{y}) = X\boldsymbol{\beta}$$
 and $V(\mathbf{y}) = \boldsymbol{\Sigma}$ and,

2.
$$E(\mathbf{y}) = \mathbf{W} \boldsymbol{\gamma}$$
 and $V(\mathbf{y}) = \boldsymbol{\Sigma}$

where X is an $n \times k$ model matrix and **W** is an $n \times q$ model matrix.

We say that one model is a **reparameterization** of the other if there is a $k \times q$ matrix F and a $q \times k$ matrix **G** such that

$$\mathbf{W} = XF$$
 and $X = \mathbf{WG}$.

The previous examples illustrate that if one model is a reparameterization of the other, then

- (i) $\operatorname{rank}(X) = \operatorname{rank}(\mathbf{W})$
- (ii) Least squares estimates of the response means are the same, i.e., $\hat{\mathbf{y}} = P_X \mathbf{y} = P_{\mathbf{W}} \mathbf{y}$
- (iii) Residuals are the same, i.e.,

$$\mathbf{e} = \mathbf{y} - \hat{\mathbf{y}} = (I - P_X)\mathbf{y} = (I - P_w)\mathbf{y}$$

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(iv) An unbiased estimator for σ^2 is provided by

$$MSE = SSE/(n - rank(X))$$

where.

$$SSE = \mathbf{e}^T \mathbf{e} = \mathbf{y}^T (I - P_X) \mathbf{y}$$
$$= \mathbf{y}^T (I - P_\mathbf{W}) \mathbf{y}$$

Reasons for reparameterizing models:

- (i) Reduce the number of parameters
 - Obtain a full rank model
 - Avoid use of generalized inverses
- (ii) Make computations easier
 - In the previous examples, $\mathbf{W}^T\mathbf{W}$ is a diagonal matrix and $(\mathbf{W}^T\mathbf{W})^{-1}$ is easy to compute
- (iii) More meaningfull interpretation of parameters.

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Result 10.

Suppose two linear models,

(1)
$$E(\mathbf{y}) = X\boldsymbol{\beta} \ V(\mathbf{y}) = \boldsymbol{\Sigma}$$

and

(2)
$$E(\mathbf{y}) = \mathbf{W}.\gamma \ V(\mathbf{y}) = \mathbf{\Sigma}$$

are reparameterizations of each other, and let Fbe a matrix such that $\mathbf{W} = XF$. Then

- (i) If $\mathbf{C}^T \boldsymbol{\beta}$ is estimable for the first model, then $\boldsymbol{\beta} = F \boldsymbol{\gamma}$ and $\mathbf{C}^T F \boldsymbol{\gamma}$ is estimable under Model
- (ii) Let $\hat{\boldsymbol{\beta}} = (X^T X)^- X^T \mathbf{y}$ and $\hat{\boldsymbol{\gamma}} = (\mathbf{W}^T \mathbf{W})^- \mathbf{W}^T \mathbf{y}$. If $\mathbf{C}^T \boldsymbol{\beta}$ is estimable, then

$$\mathbf{C}^T \hat{\boldsymbol{\beta}} = \mathbf{C}^T F \hat{\boldsymbol{\gamma}}$$

(iii) if $H_0: \mathbf{C}^T \boldsymbol{\beta} = \mathbf{d}$ is testable under one model, then $H_0: \mathbf{C}^T F \boldsymbol{\gamma} = \mathbf{d}$ is testable under the other.

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Example 24.

Consider a problem of quadratic regression in one variable, X. In particular, suppose that n=5 values of a response y are related to values x=0,1,2,3,4 by a linear model $\mathbf{y}=X\boldsymbol{\beta}+\epsilon$ for

$$\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \end{bmatrix}, \quad X = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 9 \\ 1 & 4 & 16 \end{bmatrix}, \quad \boldsymbol{\beta} = \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}, \text{ and } \boldsymbol{\epsilon} = \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \\ \epsilon_5 \end{bmatrix}$$

Define

$$\mathbf{W} = \begin{bmatrix} 1 & -2 & 2 \\ 1 & -1 & -1 \\ 1 & 0 & -2 \\ 1 & 1 & -1 \\ 1 & 2 & 2 \end{bmatrix}$$

(a) Formulate what is meant by the statement that $\mathbf{y} = \mathbf{W} \boldsymbol{\gamma} + \boldsymbol{\epsilon}$ is a reparameterization of $\mathbf{y} = X \boldsymbol{\beta} + \boldsymbol{\epsilon}$.

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- (b) Show that $\mathbf{y} = \mathbf{W}\boldsymbol{\gamma} + \boldsymbol{\epsilon}$ is reparameterization of $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$, where $\boldsymbol{\gamma}^T = [\gamma_1, \gamma_2, \gamma_3]$.
- (c) Notice that $\mathbf{W}^T\mathbf{W}$ is diagonal. Suppose that $\mathbf{y}^T = (-2,0,4,2,2)$. Find the OLS estimate of γ in the model $\mathbf{y} = \mathbf{W}\boldsymbol{\gamma} + \boldsymbol{\epsilon}$ and then OLS estimate of $\boldsymbol{\beta}$ in the original model. (Find numerical values.)

2.11 Restrictions (side conditions)

- Give meaning to individual parameters
- Make individual parameters estimable
- Create a full rank model matrix
- Avoid the use of generalized inverses
- Restrictions must involve "non-estimable" quantities for the unrestricted "effects" model.

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Example 25. An effects model

$$y_{ij} = \mu + \alpha_i + \epsilon_{ij}$$

This model can be expressed as

$$\begin{bmatrix} y_{11} \\ y_{12} \\ \vdots \\ y_{1,n_1} \\ y_{21} \\ y_{22} \\ \vdots \\ y_{2,n_2} \\ y_{31} \\ y_{32} \\ \vdots \\ y_{3,n_3} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} + \begin{bmatrix} \epsilon_{11} \\ \epsilon_{12} \\ \vdots \\ \epsilon_{1,n_1} \\ \epsilon_{21} \\ \epsilon_{21} \\ \epsilon_{22} \\ \vdots \\ \epsilon_{2,n_2} \\ \epsilon_{31} \\ \epsilon_{32} \\ \vdots \\ \epsilon_{3,n_3} \end{bmatrix}$$

Impose the restriction

$$\alpha_3 = 0$$

Then, $E(y_{1i}) =$

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$$E(y_{2j}) = E(y_{3j}) =$$
and

$$\begin{bmatrix} y_{11} \\ y_{12} \\ \vdots \\ y_{1,n_1} \\ y_{21} \\ y_{22} \\ \vdots \\ y_{2,n_2} \\ y_{31} \\ y_{32} \\ \vdots \\ y_{3,n_3} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 & 1 \\ 0 &$$

Write this model as $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$ where

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$$X = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 0 \\ 1 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 0 \end{bmatrix}$$
 and
$$\boldsymbol{\beta} = \begin{bmatrix} \mu \\ \alpha_1 \\ \alpha_2 \end{bmatrix}$$

Then, $X^TX =$ and

 $X^T \mathbf{y} =$

and the unique OLS estimator for $\boldsymbol{\beta} = (\mu \alpha_1 \alpha_2)^T$

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The unique OLS estimator for $\boldsymbol{\beta} = (\mu \ \alpha_1 \ \alpha_2)^T$

Example 26.

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Consider the model $y_{ij} = \mu + \alpha_i + \epsilon_{ij}$ with the restriction $\alpha_1 + \alpha_2 + \alpha_3 = 0$. Then, $\alpha_3 = -\alpha_1 - \alpha_2$ and

$$E(y_{1j}) = E(y_{2j}) = E(y_{3j} = and$$

$$\begin{bmatrix} y_{11} \\ y_{12} \\ \vdots \\ y_{1,n_1} \\ y_{21} \\ \vdots \\ y_{2,n_2} \\ y_{31} \\ y_{32} \\ \vdots \\ y_{3,n_3} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 1 & -1 & -1 \\ \vdots & \vdots & \vdots \\ 1 & -1 & -1 \end{bmatrix} = \begin{bmatrix} \epsilon_{11} \\ \epsilon_{12} \\ \vdots \\ \epsilon_{1,n_1} \\ \epsilon_{21} \\ \epsilon_{21} \\ \epsilon_{22} \\ \vdots \\ \epsilon_{2,n_2} \\ \epsilon_{31} \\ \epsilon_{32} \\ \vdots \\ \epsilon_{3,n_3} \end{bmatrix}$$

This model is $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$

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Example 27.

Consider the model $y_{ij} = \mu + \alpha_i + \epsilon_{ij}$ with the restriction $\alpha_1 = 0$. Then,

$$E(y_{1j}) = E(y_{2j}) = E(y_{3j})$$
and

$$\begin{bmatrix} y_{11} \\ y_{12} \\ \vdots \\ y_{1,n_1} \\ y_{21} \\ y_{22} \\ \vdots \\ y_{2,n_2} \\ y_{31} \\ y_{32} \\ \vdots \\ y_{3,n_3} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ \vdots & \vdots \\ 1 & 0 & 1 \end{bmatrix} + \begin{bmatrix} \epsilon_{11} \\ \epsilon_{12} \\ \vdots \\ \epsilon_{1,n_1} \\ \epsilon_{21} \\ \epsilon_{21} \\ \epsilon_{22} \\ \vdots \\ \epsilon_{2,n_2} \\ \epsilon_{31} \\ \epsilon_{32} \\ \vdots \\ \epsilon_{3,n_3} \end{bmatrix}$$

This model is $\mathbf{y} = X\boldsymbol{\beta} + \boldsymbol{\epsilon}$, with

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 $X = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 1 & 0 \\ \vdots & \vdots & \vdots \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 1 & 0 & 1 \\ \vdots & \vdots & \vdots \\ 1 & 0 & 1 \end{bmatrix}$ and $\boldsymbol{\beta} = \begin{bmatrix} \mu \\ \alpha_2 \\ \alpha_3 \end{bmatrix}$

The unique OLS estimator for $\boldsymbol{\beta} = (\mu \ \alpha_1 \ \alpha_2)^T$ is

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The restrictions (i.e. the choice of one particular solution to the normal equations) have no effect on the OLS estimates of estimable quantities. The estimated treatment means are:

$$\begin{split} E(\hat{y}_{1j}) &= \hat{\mu} = \bar{y}_{1.} \\ E(\hat{y}_{2j}) &= \hat{\mu} + \hat{\alpha}_{2} = \bar{y}_{2.} \\ E(\hat{y}_{3j}) &= \hat{\mu} + \hat{\alpha}_{3} = \bar{y}_{3.} \end{split}$$